

Table from

***pK<sub>a</sub> values in organic chemistry – making maximum use of the available data***

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*Tetrahedron Letters* **2018**, <https://doi.org/10.1016/j.tetlet.2018.08.054>

Table 5. Examples of absolute and relative pK<sub>a</sub> values of neutral and cationic acids in some solvents from refs <sup>11,15,16,18,25,41,45–52</sup>. All values are experimental unless noted otherwise.<sup>a</sup>

	MeCN	DCE	DMSO	H <sub>2</sub> O	THF	C7	DME
Absolute pK <sub>a</sub> values	Picric acid	11.00	44.6	-1.0	0.3	11.84	
	C(CN) <sub>2</sub> =C(CN)OH	4.69	35.9				
	(2-C <sub>10</sub> F <sub>7</sub> ) <sub>2</sub> CHCN	19.32	53.0			-0.68	
	(C <sub>6</sub> F <sub>5</sub> ) <sub>2</sub> CHCN	21.10	55.7 <sup>b</sup>	8.0		1.80	6.4
	9-C <sub>6</sub> F <sub>5</sub> -Octafluorofluorene	18.88	53.8			0.00	5.3
	(4-CF <sub>3</sub> -C <sub>6</sub> F <sub>4</sub> )(C <sub>6</sub> F <sub>5</sub> )CHCN	18.14	52.3	4.9		-1.39	3.9
	(C <sub>6</sub> H <sub>5</sub> )(C <sub>6</sub> F <sub>5</sub> )CHCN	26.14		12.8			11.8
	Saccharin	14.57		4.0	1.8		
	2,4-(NO <sub>2</sub> ) <sub>2</sub> -Phenol	16.66		5.4	4.10	16.94	
	HCl	10.30	45.2	-2.0 <sup>c</sup>	-5.9 <sup>c</sup>		
	HBr	5.5	40.6	-6.8 <sup>c</sup>	-8.8 <sup>c</sup>		
	HI	2.8	37.7	-10.9 <sup>c</sup>	-9.5 <sup>c</sup>		
	HClO <sub>4</sub>	1.83	32.2	-14.9 <sup>c</sup>	-15.2 <sup>c</sup>	7.57	
	TfOH	2.60	33.7	-14.3 <sup>c</sup>	-14.7 <sup>c</sup>	7.83	
	Acetic acid	23.51		12.6	4.75	22.48	
	Benzoic acid	21.51		11.1	4.25	25.11	
	Aniline-H <sup>+</sup>	10.62		3.59	4.60	5.2	
	Pyridine-H <sup>+</sup>	12.53		3.45	5.25	5.5	
	Proton Sponge-H <sup>+</sup>	18.62		7.47		11.1	
	DBU-H <sup>+</sup>	24.34		13.9		16.6	
	TBD-H <sup>+</sup>	26.03				19.4	
	<i>t</i> -BuP <sub>1</sub> (dma) <sub>3</sub> -H <sup>+</sup>	26.98		15.7		18.8	
	<i>t</i> -BuP <sub>1</sub> (pyrr) <sub>3</sub> -H <sup>+</sup>	28.42				20.2	
	Et <sub>3</sub> N-H <sup>+</sup>	18.63		9.0	10.70	12.5	
	TMG-H <sup>+</sup>	23.30		13.2	13.60	15.5	
Relative pK <sub>a</sub> values	Picric acid – C(CN) <sub>2</sub> =C(CN)OH	6.31	8.70				
	(2-C <sub>10</sub> F <sub>7</sub> ) <sub>2</sub> CHCN – Picric acid	8.32	8.40				
	(2-C <sub>10</sub> F <sub>7</sub> ) <sub>2</sub> CHCN – C(CN) <sub>2</sub> =C(CN)OH	14.63	17.10				
	Saccharin – Picric acid	3.57		5.00	1.50		
	2,4-(NO <sub>2</sub> ) <sub>2</sub> -Phenol – Saccharin	2.09		1.40	2.30		
	2,4-(NO <sub>2</sub> ) <sub>2</sub> -Phenol – Picric acid	5.66		6.40	3.80	5.1	
	(C <sub>6</sub> F <sub>5</sub> ) <sub>2</sub> CHCN – (4-CF <sub>3</sub> -C <sub>6</sub> F <sub>4</sub> )(C <sub>6</sub> F <sub>5</sub> )CHCN	2.96	3.4	3.10		3.19	2.50

(C <sub>6</sub> F <sub>5</sub> ) <sub>2</sub> CHCN –	2.22				1.80	1.10
9-C <sub>6</sub> F <sub>5</sub> -Octafluorofluorene						
(2-C <sub>10</sub> F <sub>7</sub> ) <sub>2</sub> CHCN –	0.44	-0.80			-0.68	
9-C <sub>6</sub> F <sub>5</sub> -Octafluorofluorene						
Picric acid – HCl	0.70	-0.60	1.00	6.20		
Picric acid – HBr	5.50	4.00	5.80	9.10		
Picric acid – HI	8.20	6.90	9.90	9.80		
HCl – HI	7.50	7.50	8.90	3.60		
HCl – HClO <sub>4</sub>	8.47	13.00	12.90	9.30		
HCl – TfOH	7.70	11.50	12.30	8.80		
TfOH – HClO <sub>4</sub>	0.77		0.6	0.5	0.26	
Acetic acid - Picric acid	12.51		13.60	4.45	10.54	
Benzoic acid - Picric acid	10.51		12.10	3.95	13.17	
Acetic acid - Benzoic acid	2.00		1.50	0.50	2.63	
Benzoic acid - HCl	11.21		13.10	10.15		
DBU-H <sup>+</sup> – Proton Sponge-H <sup>+</sup>	5.72		6.4		5.50	
Proton Sponge-H <sup>+</sup> – Pyridine-H <sup>+</sup>	6.09		4.0		5.60	
Pyridine-H <sup>+</sup> – Aniline-H <sup>+</sup>	1.91		-0.1	0.65	0.30	
Proton Sponge-H <sup>+</sup> – Aniline-H <sup>+</sup>	8.00		3.9		5.90	
DBU-H <sup>+</sup> – Pyridine-H <sup>+</sup>	11.81		10.5		11.10	
DBU-H <sup>+</sup> – Aniline-H <sup>+</sup>	13.72		10.3		11.40	
<i>t</i> -BuP <sub>1</sub> (pyrr) <sub>3</sub> -H <sup>+</sup> – DBU-H <sup>+</sup>	4.08				3.60	
<i>t</i> -BuP <sub>1</sub> (dma) <sub>3</sub> -H <sup>+</sup> – DBU-H <sup>+</sup>	2.64		1.8		2.20	
<i>t</i> -BuP <sub>1</sub> (pyrr) <sub>3</sub> -H <sup>+</sup> – TBD-H <sup>+</sup>	2.39				0.80	
<i>t</i> -BuP <sub>1</sub> (dma) <sub>3</sub> -H <sup>+</sup> – TBD-H <sup>+</sup>	0.95				-0.60	
Et <sub>3</sub> N-H <sup>+</sup> – Pyridine-H <sup>+</sup>	6.10		5.5	5.45	7.00	
Et <sub>3</sub> N-H <sup>+</sup> – Aniline-H <sup>+</sup>	8.01		5.4	6.10	7.30	
<i>t</i> -BuP <sub>1</sub> (dma) <sub>3</sub> -H <sup>+</sup> - TMG-H <sup>+</sup>	3.68		2.50		3.30	
DBU-H <sup>+</sup> - TMG-H <sup>+</sup>	1.04		0.70		1.10	

<sup>a</sup> Abbreviations and acronyms: **C7** is Heptane; TfOH [1493-13-6] is trifluoromethanesulfonic acid, CF<sub>3</sub>SO<sub>3</sub>H; Picric acid is 2,4,6-trinitrophenol; Proton Sponge [20734-58-1]; DBU [6674-22-2]; TBD [5807-14-7]; *t*-BuP<sub>1</sub>(pyrr) [161118-67-8]; *t*-BuP<sub>1</sub>(dma) [81675-81-2]; TMG [80-70-6]. <sup>b</sup> The pK<sub>a</sub> value actually corresponds to the compound (4-C<sub>6</sub>F<sub>4</sub>)(C<sub>6</sub>F<sub>5</sub>)CHCN but it is expected to be very similar. <sup>c</sup> Computational values from ref 2.